



Figure 8. Complex oscillatory patterns: the three-dimensional limit cycle $(\alpha, \beta, \text{ and } z).$

variable—the concentration x of the dimer B_2 . Gaspar and Showalter⁹ have invoked such a scheme for oscillations in the Landolt reaction.

What is no less remarkable is the versatile behavior of the three-variable model. While the particular scheme chosen (E_0) $\neq 0, Q_2 \neq 0$) may at first seem special, it is indeed the removal of an autocatalytic species that is likely to be most exothermic and the generation of species A that is most likely to have a normal activation energy ("normal" means large compared with RT_a). The behavior found is probably widely representative. Yet this simple model shows period doubling to chaos (without any forcing

(9) Gaspar, V.; Showalter, K., 1989, personal communication.

terms and with the minimum number of variables). It also offers complex oscillations of a very different kind, at least superficially resembling those encountered in hydrocarbon oxidation.¹⁰ Some authors have called these "mixed mode" oscillations, but that term seems more appropriate when the attractor is a simple torus. Our attractor is not such, and we propose that the answer is more like motion on the surface of a lemon. Small excursions correspond to limit cycles around the nipple and large ones to limit cycles around the body of the fruit. However, the surface is not really a body of revolution, so the metaphorical answer is not quite a lemon.

It is notable that the channel that has been opened for thermal feedback does not require the strong nonlinearity usually associated with self-heating effects. Complexities persist even into the linear region of feeble thermal feedback: merely opening the channel is enough.

Expected values for the parameter ζ (Zel'dovich number) are important. The constituent (RT_a^2/E) may reasonably be 10-20 K. The self-heating possible if all P is converted to C adiabatically may be from 0 to 2000 K in a gas reaction and from 0 to 20 K in molar solution. However, this large span is reduced in the ratio of $a_{\rm rf}$ to p_0 (which is of order k_0/k_2)—say by $10^{-2}-10^{-3}$ —so we are talking about temperature effects from 0 to 20 K in a gas and from 0 to 200 mK in a solution (when ζ is easily 0.01 or less). Such effects are more likely to be present than not: at the very least they require attention.

Acknowledgment. We thank the SERC and Gonville & Caius College, Cambridge, for support. We are also grateful to Dr. Scott and Miss Tomlin of Leeds and Dr. Needham of East Anglia for lively discussion.

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A Two-Fluid Model for Turbulent Diffusion Flames at Moderate Damköhler Numbers

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Since most practical combustors involve turbulent, nonpremixed flames, research has focused on developing a fundamental understanding of such flames. In the present paper, the oxidation of carbon monoxide by air in a turbulent flow is investigated. The turbulent reacting flow is described adopting Spalding's intermittency model, the two-fluid model, which was developed to improve the modeling of exchange processes within the turbulent mixing layer of the two gas streams. The turbulent flow field is modeled adopting a classical $k-\epsilon$ turbulence model. Since the oxidation of carbon monoxide at moderate Damköhler numbers cannot be considered as being diffusion controlled, the two-fluid model is extended to include the finite reaction rate adopting a global rate expression. The reaction model is closed by using a three-dimensional probability density function with respect to the mixture fraction, the mass fraction of carbon monoxide, and enthalpy. The results of the calculations are compared with results from a corresponding single-fluid model as well as results of measurements in a turbular furnace 5 m in length and 0.5 m in diameter which clearly show an improvement of the simulations of the turbulent diffusion flame with the two-fluid model compared to the single-fluid calculations within the turbulent mixing layer.

Introduction

Turbulent diffusion flames are characterized by their strong coupling between the turbulent mixing of the fuel and the oxidizer and the chemical reactions. In a great class of combustion processes turbulent mixing determines combustion. In this case the transport equations for the turbulent flow field and a conserved scalar are solved.1 One recent development of the conserved scalar approach are the "flamelet models",^{2,3} which are applied successfully to systems with fast chemistry. Combustion systems involving reactions that are not or not completely controlled by the turbulent mixing necessitate the explicit description of the chemical reaction rate which has to be formulated with respect to the turbulent character of the flow. The approach followed

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⁽¹⁾ Bilger, R. W. In Turbulent Reacting Flows; Libby, P. A., Williams,

<sup>F. A., Eds.; Springer: New York, 1980; p 65.
(2) Williams, F. A. In</sup> *Turbulent Mixing in Nonreactive and Reactive Flows*; Murthy, S. N. B., Ed.; Plenum Press: New York, 1975; p 189.

⁽³⁾ Peters, N. Prog. Energy Combust. Sci. 1984, 10, 319.

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in the present work describes the mean turbulent reaction rate using a probability density function (pdf) closure, where the instantaneous chemical reaction rate is weighted by a multidimensional probability density function.4,5

Considering chemical reactions in a turbulent flow either at high Damköhler numbers or at moderate Damköhler numbers requires the modeling of coherent structures which may occur at the edge of the turbulent jet, and of intermittency. (The Damköhler number is defined as the ratio of the mixing time and a characteristic time for the chemical reaction.) Spalding⁶ initiated an intermittency model defining two distinguished phases (not in the physical sense), laminar (oxidant rich) and turbulent (fuel rich); this formulation refers to the situation in a turbulent free jet. The model was developed to improve the mathematical description of the exchange processes at the interface of the two phases.

The scope of the present investigation is the extension of Spalding's two-fluid model to turbulent reacting flows at moderate Damköhler numbers. The oxidation of carbon monoxide by air in a turbulent flow is evaluated as model reaction, since this reaction is the rate-controlling step in all carbon-containing combustion processes. The results of the calculations with the two-fluid model are compared with results of a corresponding one-fluid model as well as experimental data.

The Experiment

A mixture of nitrogen and ca. 9% carbon monoxide was admixed axially through a nozzle 10 mm in diameter into the completely burnt flue gas of a natural gas flame which was operated with excess air. Considering the two-fluid model, the fuel-rich gas stream is treated as the turbulent phase the Reynolds number of which is 6970 for the simulated test series. The completely burnt flue gas of the natural gas flame which is oxidant-rich is considered as being laminar. For details of the experimental setup and the measurements see refs 7 and 8.

The Mathematical Model

Following Spalding's principal suggestion⁶ and the work of Malin⁹⁻¹¹ and Markatos et al.,¹² the two-fluid model distinguishes a turbulent phase which carries the fuel, the reaction products, and the entrained oxidant, and a phase which is treated as laminar comprising the oxidant. This model requires the formulation of conservation equations for all variables governing the turbulent flow field as well as mass fractions for the chemical species for each phase. In order to describe the interchange processes between the two phases, a variable r_i is defined which can be interpreted as the presence probability of phase *i*, the volume fraction, or the intermittency factor of phase *i*. In addition, the turbulent fluctuations for the variables of the turbulent phase, say phase 1, have to be modeled for the turbulent flow field as well as for the turbulent reaction rate and the concentrations of chemical species.

In general, the transport equation for the Reynolds average ϕ_i of a variable ϕ_i of phase *i* presuming a conventional eddy viscosity gradient model of turbulent transport can be formulated as^{9,12} The Journal of Physical Chemistry, Vol. 94, No. 8, 1990 3309

The variable $\overline{\phi}_i$ stands for either a flow field variable, for enthalpy, or for the mass fraction of a chemical species. All other values appearing in eq I will be specified in the next two sections.

1. Modeling the Turbulent Flow Field. Modeling the turbulent flow field for a two-dimensional, axisymmetrical, parabolic flow, the transport equations for the volume fractions r_i and for the velocity components w_i in the main flow direction and v_i in the radial direction have to be formulated. Since the first phase is treated as turbulent, the Reynolds stresses for this phase have to be modeled as well. In the present investigation a conventional $k-\epsilon$ model is adopted, where k denotes the turbulent kinetic energy and ϵ its rate of dissipation. The applicability of the turbulence model will be demonstrated by modeling an inert test series.

The first term in eq 1 is zero for steady flows, the second and third terms describe the convective and diffusive transport of variable ϕ_i where the exchange coefficients are formulated as in the single-fluid model.^{4,5} The last term of the left-hand side describes phase diffusion^{9,10,12} at the turbulent/nonturbulent interface. The diffusivity D_y is described by¹²

$$D_{y} = k_{s}\bar{\rho} \left| \frac{\partial \bar{w}}{\partial y} \right| \Lambda^{2}$$
⁽²⁾

where \bar{w} is the mean velocity of the mixture in the main flow direction which prevails in parabolic situations, $\bar{\rho}$ is the phase averaged density, y is the coordinate in radial direction, and k_s equals 0.65.¹² In eq 2 the turbulent fragment size is calculated from the turbulence quantities k and ϵ :¹²

$$\Lambda = c_{\rm D}^{3/4} (\bar{k}^{3/2}/\bar{\epsilon}) \tag{3}$$

 $c_{\rm D}$ is a standard parameter which equals 0.09.^{13,14} Considering the conservation equations of the phase volume fractions, the intraphase sources \bar{S}_{ϕ_i} are zero whereas the interphase source \bar{I}_{r_1}

$$\bar{I}_{r_1} = \dot{E}^{\prime\prime\prime} = k_m \bar{r}_1 \bar{r}_2 \bar{\rho}_2 |\bar{W}_1 - \bar{W}_2| / \Lambda \tag{4}$$

accounts for interfluid mass transfer per unit volume from the laminar to the turbulent phase (engulfment); here $|\bar{W}_1 - \bar{W}_2|$ is the difference in total velocity and k_m equals 0.35.9.12 The intrasource terms for momentum equations equal the source terms that usually appear as sources in the Navier-Stokes equations. Considering the turbulence quantities k and ϵ , the standard intraphase source terms as well as widely used standard parameters are adopted.^{13,14} The interphase sources for k and ϵ are zero, since these variables belong to the turbulent phase. Malin¹⁰ proposed a modified form of the $k-\epsilon$ model for two-fluid situations which does not produce significant differences in the results compared with the standard model for the present application. Therefore, the standard model is applied.

Following Malin9-11 and Markatos,15 the interphase sources for the remaining first phase variables are

$$\bar{I}_{\phi_1} = \bar{\phi}_2 \dot{E}^{\prime\prime\prime} - F_{\phi} \tag{5}$$

with

$$F_{\phi} = k_{\phi} \bar{r}_1 \bar{r}_2 \bar{\rho}_2 |\bar{W}_1 - \bar{W}_2| (\bar{\phi}_1 - \bar{\phi}_2) / \Lambda \tag{6}$$

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 F_{ϕ} describes the interfluid friction forces per unit mass arising from the different velocity between the two fluids. Interphase sources for variables belonging to the second phase are $\bar{I}_{\phi_2} = -\bar{I}_{\phi_1}$. For velocities in eq 6 k_{ϕ} equals 0.05.^{9,12} In the one-phase problem, the turbulent Prandtl-Schmidt numbers of the variables f, Y_{CO} , and h are 0.7; this means that the exchange of these variables is 1/0.7 times faster than the exchange of momentum. Therefore, the constants k_f , $k_{Y_{CO}}$, and k_h are taken as 0.0714, which almost equals 0.1, the value Malin⁹ proposed for the corresponding constant for temperature. All employed constants have been used as standard parameters, so that the model is not restricted to the present application.

2. Modeling the Chemical Reactions. The oxidation of carbon monoxide by air is described by a global rate expression¹⁶

$$\dot{w}_{co} =$$

$$-3.98 \times 10^{17} \rho^{1.75} Y_{\rm CO} \left(\frac{Y_{\rm H_{2}O}}{M_{\rm H_{2}O}} \right)^{0.5} \left(\frac{Y_{\rm O_2}}{M_{\rm O_2}} \right)^{0.25} \exp \left(-\frac{20\,000}{T} \right)$$
(7)

where \dot{w}_{CO} is given in kg m⁻³ s⁻¹, ρ in g cm⁻³, and the temperature, T, in kelvin. Here Y_i denotes the mass fraction of species i and M_i its molecular weight in g mol⁻¹. This kinetic rate expression may be reduced to $\dot{w}_{CO} = \dot{w}_{CO}(f, Y_{CO}, h)$, since water can be treated as inert.^{4,5} Here f denotes mixture fraction, Y_{CO} the mass fraction of carbon monoxide, and h enthalpy.

According to the principles of pdf closure,^{5,17} and considering that only variables of the first phase fluctuate, the mean turbulent reaction rate is formulated as

$$\overline{\dot{w}_{\rm CO}} = \frac{1}{Z} \int_{h_1, \rm in}^{h_2, \rm in} \int_0^1 \int_0^1 \dot{w}_{\rm CO}(f_1, f_2, Y_{\rm CO,1}, Y_{\rm CO,2}, h_1, h_2) \times P(f_1, Y_{\rm CO,1}, h_1) \, df_1 \, dY_{\rm CO,1} \, dh_1$$
(8)

where Z is a normalization factor due to the density of the applied pdf.^{4,5} The instantaneous reaction rate is formulated in dependence of the phase-averaged values of the two phases.

The probability density function $P(f_1, Y_{CO,1}, h_1)$ is formulated by using a three-dimensional Gaussian distribution, because this distribution includes influences of variances as well as covariances of its dependent variables on the turbulent reaction rate.^{4,5} The importance of including nonzero covariances in the reaction model has also been demonstrated by Pope and Correa.¹⁸ Since the discussion of the principles of the joint pdf approach as well as its effect on the turbulent reaction rate is available from refs 4 and 5, the present paper focuses on the formation of the joint pdf closure for the two-fluid model. The shape of the joint Gaussian distribution is determined in dependence of the means, variances, and covariances of the first-phase variables f_1 , $Y_{CO,1}$, and h_1 which are calculated from conservation equations, and thus the shape of the pdf varies in accordance to the situation prevailing within the turbulent flow field. The intraphase sources for the mean values of f, Y_{CO} , and h are given by eq 5; eq 8 is the interphase source term for Y_{CO} , whereas interphase sources for all other mean values are zero. The mean values for the second-phase variables need to be solved in order to satisfy the total mass balance. The reaction rate of the oxidation of carbon monoxide in the second phase is zero, since reaction occurs only in the first phase. The variances and covariances for f_1 , Y_{CO_1} , and h_1 are calculated from

$$L(\phi'_{1i}\phi'_{1j}) = c_1\eta_i\frac{\partial\bar{\phi}_{1i}}{\partial x_k}\frac{\partial\bar{\phi}_{1j}}{\partial x_k} - c_2\bar{\rho}_1\frac{\bar{\epsilon}}{\bar{k}}\overline{\phi'_{1i}\phi'_{1j}} + \overline{\phi'_{1i}S'_{\phi_{1j}}} + \overline{\phi'_{1j}S'_{\phi_{1i}}} (9)$$

The last two terms on the right-hand side of eq 9 are determined

following the principles of pdf closure:

$$\overline{\phi'_{1i}S'_{\phi_{1j}}} = \frac{1}{Z} \int_{h_{1,\text{in}}}^{h_{2,\text{in}}} \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} (\phi_{1i} - \bar{\phi}_{1i}) \times (S_{\phi_{1j}} - \bar{S}_{\phi_{1j}}) P(f_{1}, Y_{\text{CO},1}, h_{1}) \, \mathrm{d}f_{1} \, \mathrm{d}Y_{\text{CO},1} \, \mathrm{d}h_{1}$$
(10)

To achieve closure of the system of partial differential equations, the temperature of each phase is calculated from the caloric equation of state, and the density of each phase is calculated from the ideal-gas equation of state.

The system of partial differential equations has been solved by using a numerical procedure for multiphase flows developed by Spalding et al.,¹⁹ which is available in the computer code PHOENICS-84.20 In order to obtain convergence, relaxation with "false time steps" was adopted. In addition, convergence in the initial development region of the jet has been achieved by restricting the changes of entrainment and interphase friction to 50% for each iteration.

Results and Discussion

The results of the calculations on the one hand are compared with experimental data, and on the other hand they are compared with the corresponding one-fluid model,⁵ where the problem is simulated by adopting the $k-\epsilon$ turbulence model and the joint pdf closure.

1. Results of the Two-Fluid Calculations. At first, calculations were performed for a test series, where pure nitrogen was admixed into the hot, turbulent flue gas of the natural gas flame in order to check the validity of the $k-\epsilon$ turbulence model and the employed standard parameters. Figure 1 displays results of the calculated and measured radial profiles of temperature, velocity in main flow direction, and the volume fraction of oxygen at a distance of 0.16 m from the exit nozzle. The agreement between measurements and calculations is reasonably good, so that calculations with chemical reactions were performed applying standard parameters throughout.

Figure 2 shows axial and radial profiles for the turbulence quantities k, ϵ , and the effective viscosity at a distance of 0.16 m from the nozzle plain for a test series the inlet conditions of which are given below the figure. The profiles are not compared with experimental data which are not available for the test series. Nevertheless, they give some insight in the situation of the considered turbulent flow field. The turbulent reaction zone extends the distance of 0.05-0.2 m from the nozzle exit. In the radial direction, the quantities fall to zero because all field variables belong to the first turbulent phase, which is present only near the axis. Figure 3 shows the volume fractions of the two fluids and the rate of entrainment at distances of 0.16 and 0.63 m from the exit nozzle. The presence probability of the fuel stream is unity near the axis; at greater distances from the axis pure oxidant is present. Obviously, the entrainment of laminar fragments proceeds at greater distances from the exit nozzle as well as at greater distances from the axis. The maximum of entrainment lies within the turbulent mixing zone of the two phases.

In order to compare the results of the calculations with experimental data, the following figures display radial profiles at a distance of 0.16 m from the nozzle plain; this is the place lying within the turbulent reaction zone (cf. Figure 2). Figure 4 shows a comparison of measured and calculated radial profiles of temperature and volume fractions of oxygen and carbon monoxide. In general the experimental data are well predicted by the twofluid model. At the axis the calculated values of temperature are higher than the measured data leading to volume fractions of carbon monoxide that lie below the measurements according to the exponential temperature dependence of the kinetic rate expression (cf. eq 7) which is only valid for temperatures higher than 800 K.²¹ Fuel enters the combustion chamber with a temperature

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Figure 1. Comparison of calculated and measured profiles of temperature, velocity in main flow direction, and volume fraction of oxygen. Experimental conditions: $T_{fu,in} = 825$ K, $Y_{CO,in} = 0$, $Re_{fu,in} = 6800$, $T_{ox,in} = 1090$ K, $Y_{ox,in} = 0.1303$, $Re_{ox,in} = 3900$.



Figure 2. Calculated profiles of the turbulence quantities k, ϵ , and η_{eff} . Experimental conditions: $T_{\text{fu,in}} = 790 \text{ K}$, $Y_{\text{CO,in}} = 0.0909$, $\text{Re}_{\text{fu,in}} = 6970$, $T_{\text{ox,in}} = 1050 \text{ K}$, $Y_{\text{ox,in}} = 0.1427$, $\text{Re}_{\text{ox,in}} = 3990$.

of 790 K; therefore, the calculated temperature at the axis lies above the measured value.

2. Comparison of the Two-Fluid Calculations with the One-Fluid Model. Finally the results obtained with the two-fluid model are compared with results of a corresponding one-fluid model. Figure 5 shows radial profiles of the volume fractions of carbon monoxide at a distance of 0.16 m from the exit nozzle for two different test series the conditions of which are given below the figure. The upper part of the figure displays a comparison of the experimental results with results of calculations including the two-fluid model, and the lower part displays the results of the



Figure 3. Calculated profiles of the volume fractions of the phases and entrainment. Experimental conditions as in Figure 2.



Figure 4. Comparison of calculated and measured profiles of temperature and volume fractions of carbon monoxide and oxygen. Experimental conditions as in Figure 2.

experiments and the one-fluid model. Near the axis the two different models produce the same results. In this region the turbulent phase is present with probability one (cf. Figure 3); hence the two-fluid model satisfies the one-fluid conditions. At greater distances from the axis the one-fluid model calculates lower profiles of carbon monoxide volume fractions. The differences arise within the turbulent mixing zone of the two phases; this is between 0.02 and 0.055 m from the axis (cf. Figure 3), where the turbulent jet may be effected by "coherent structures" and intermittency. The influence of turbulent fluctuations of the field variables determining the turbulent flow field as well as the fluctuations of the chemical species is overpredicted by the one-fluid model, leading to overestimated exchange between the phases and to an overpredicted reaction rate. In this region, the one-fluid model does not consider effects of intermittency causing lower fluctuations for instance of temperature which cause a retardation of the turbulent reaction.⁵ The discrepancies between the measured and

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Figure 5. Comparison of calculated profiles of carbon monoxide volume fractions with the two-fluid model (upper part) and the single-fluid model (lower part) and measured data. Experimental conditions: (O) as in Figure 2, (Δ) $T_{fu,in} = 830$ K, $Y_{CO,in} = 0.0909$, $\text{Re}_{fu,in} = 6770$, $T_{ox,in} = 1100$ K, $Y_{ox,in} = 0.1248$, $\text{Re}_{ox,in} = 3920$.

calculated profiles at about 0.05–0.06 m from the axis also might be due to uncertainties in measuring very small values of carbon monoxide mass fractions or to effects of chemical nonequilibrium which are not considered by adopting an irreversible one-step mechanism. However, a comparison between measurements and calculations shows a significant improvement of the simulations adopting the two-fluid model especially in the region of the turbulent mixing at the turbulent/nonturbulent interface. For both test series the profiles of the volume fractions of carbon monoxide are well predicted by the two-fluid model.

Conclusions

The oxidation of carbon monoxide by air in a turbulent flow at moderate Damköhler numbers has been modeled by adopting a two-fluid model distinguishing a turbulent fuel-rich and a laminar oxidant-rich phase. The turbulent flow field has been described applying an eddy-viscosity gradient model of turbulent transport and a conventional $k-\epsilon$ turbulence model for the turbulent phase. The chemical reactions have been modeled by adopting a global rate expression and a multivariate pdf approach. The results of the two-fluid calculations were compared with corresponding one-fluid simulations and with experimental data. The two-fluid calculations show a significant improvement in predicting the experimental data compared with the one-fluid predictions. The differences between the model calculations arise within the turbulent mixing zone of the fuel and the oxidizer; this is the region where also chemical reactions take place. The agreement of the simulations of the two-fluid model with the experimental results is good for all field variables.

An improvement of the model may be achieved by including more complex chemistry such as reduced mechanisms. In this case, mass conservation equations for the additional species need to be solved for both phases the formulation of which corresponds to the one given here for the reactive species CO. The mean chemical reaction rate for the additional species (compare eq 8), however, needs to be revised due to the different rate expression, and the joint pdf has to involve the dependent variables of the employed kinetic rate expression.

Acknowledgment. The author wishes to thank Professor F. Fetting for his sustained interest in this work. She thanks Professor D. B. Spalding from CHAM Ltd., London, for many helpful discussions and for the computer code PHOENICS-84. The financial support of the Stiftung Volkswagenwerk is gratefully acknowledged.

Registry No. CO, 630-08-0.